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EQUATION OF STATES OF THE POTTS FERROMAGNET IN ANISOTROPIC SQUARE LATTICE: RENORMALIZATION GROUP APPROACH

by

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ABSTRACT

We extend to the anisotropic case (not necessarily equal coupling constants along the various crystalline directions) the real space renormalization group procedure recently introduced by Caride and Tsallis, which directly yields the order parameter for arbitrary temperatures. The method does not demand the calculation of the thermodynamic energy, it is as simple as a mean field calculation although it provides non trivial results, which can be systematically improved. Within the present extension, the coordination number of any given site is generalized into a suitable average of the coupling constants involving that site. We apply the procedure to the q-state Potts ferromagnet in anisotropic square lattice, whose exact equation of states is still unknown. Whenever possible, the results compare satisfactorily with available exact results.

Key-words: Potts model; Renormalization group; Equation of states; Anisotropic square lattice.

1 INTRODUCTION

Real space renormalization group (RG) techniques have been largely employed to evaluate critical points (phase diagrams) and critical exponents. In general, these procedures have been used to derive relevant quantities in the *vicinity* of the critical points. There is, however, no fundamental reason for not using these techniques far from the critical region, especially if we are looking for approximate results. Indeed RG formalisms are available[1,2] for calculating the relevant thermodynamic energy for *arbitrary* values of the external parameters (temperature, magnetic field, etc.); from it, quantities such as the specific heat, equation of states and susceptibility, can be obtained through the standard thermodynamical relations.

It has been recently introduced[3] a RG formalism that enables the (direct) calculation of equations of states for *geometrical* statistical systems, which cannot be described within a Hamiltonian framework. Along the same lines, Caride and Tsallis[4] have now proposed a RG method which allows, for *thermal* statistical systems, the *direct* calculation (without going through the calculation of the thermodynamic energy) of the equation of states for arbitrary values of the external parameters. The system which was focused by Caride and Tsallis is an *isotropic* one in which the coupling constants involved on every site are one and the same. Consequently the coordination number plays an important role since the order parameter is locally proportional to this number (in fact, within this type of approach the Bravais lattice, translationally invariant, is approximated by a suitable hierarchical lattice, scale invariant). In the present paper, we extended the formalism to *anisotropic* systems; within this extension the coordination number is generalized

into a natural average of the coupling constants involved in any given site. As an application of this procedure we calculate an approximation for the still unknown spontaneous order parameter of the q-state Potts ferromagnet in anisotropic square lattice (arbitrary coupling constants J_x and J_y). The q-dependence (exactly known) of the critical exponent β and the q- and J_y/J_x-dependences (still unknown for $q\neq 2$) of the critical amplitude are particularly focused.

In Section II we present the formalism and its application to the Potts model; in Section III we present the results, and finally conclude in Section IV.

II FORMALISM AND MODEL

We consider a d-dimensional simple cubic lattice of linear size L, and assume that first-neighboring sites interact ferromagnetically, the d (dimensionless) coupling constants being $K_\alpha=J_\alpha/k_BT$ ($\alpha=x,y,z,...$), where $J_\alpha \geq 0$ is the coupling constant along the α-axis and refers to Ising, xy, Heisenberg, Potts models or similar ones. Whenever ordering of the coupling constants becomes convenient we shall use the convention $J_x \geq J_y \geq J_z \geq ...$

The order parameter M is defined as $M \equiv N_L(K_x,K_y,K_z,...)/L^d$ in the $L \to \infty$ limit, where $N_L(K_x,K_y,K_z,...)$ is the thermal average number of sites whose spin is pointing along the easy magnetization direction (for instance, the $\sigma_i=1$ state for the Potts ferromagnet) minus those whose spin is pointing in the other directions (i.e., $\sigma_i=2,...,q$). We associate with each site of the lattice an elementary dimensionless magnetic dipole μ, which will be a renormalization

variable of our transformation.

We renormalize the original system into a system of linear size L' ($B \equiv$ linear expansion factor $= L/L' > 1$) and associate to the new system the renormalized variables K'_x, K'_y, K'_z,... and μ', which will depend on K_x, K_y, K_z,... and μ. Through renormalization the *total magnetic moment of the system must be preserved*, i.e.

$$N_{L'}(K'_x,K'_y,K'_z,\ldots)\mu' = N_L(K_x,K_y,K_z,\ldots)\mu \tag{1}$$

We now divide both sides by L^d and obtain

$$M(K'_x,K'_y,K'_z,\ldots)\mu' = M(K_x,K_y,K_z,\ldots)\mu B^d \tag{2}$$

where $M(K'_x,K'_y,K'_z,\ldots) \equiv N_{L'}(K'_x,K'_y,K'_z,\ldots)/L'^d$. If we start with K_x, K_y, K_z,... and $\mu^{(o)}$ and iterate n times we obtain

$$M(K_x^{(n)},K_y^{(n)},K_z^{(n)},\ldots)\mu^{(n)} = M(K_x,K_y,K_z,\ldots)\mu^{(o)}B^{nd}$$

which yields, in the $n \to \infty$ limit,

$$M(K_x,K_y,K_z,\ldots) = \lim_{n\to\infty} \frac{M(K_x^{(n)},K_y^{(n)},K_z^{(n)},\ldots)\mu^{(n)}}{B^{nd}} \tag{3}$$

where we have arbitrarily chosen $\mu^{(o)}=1$.

Together with Eq. (3) we will use the RG recurrence equations for $\{K'_\alpha\}$. These equations will typically give rise to a critical frontier in the d-dimensional parameter space. This critical surface will partition the space in two (or more) phases, namely the disordered phase (paramagnetic) attracted, under renormalization, by the stable fixed point $K_x=K_y=K_z=\ldots=0$, and the ordered phase

(ferromagnetic) attracted, under renormalization, by the stable fixed point $K_x = K_y = K_z = \ldots \to \infty$. In the paramagnetic region we have that $M(K_x^{(\infty)}, K_y^{(\infty)}, K_z^{(\infty)}, \ldots) = 0$, which, through Eq. (3), implies $M(K_x, K_y, K_z, \ldots) = 0$ (we shall verify later on that $\lim_{n\to\infty} \frac{\mu^{(n)}}{B^{nd}}$ does not diverge). On the other hand, in the ferromagnetic region we have that $M(K_x^{(\infty)}, K_y^{(\infty)}, K_z^{(\infty)}, \ldots) = 1$ (conventional value for the order parameter of the completely ordered system), and consequently

$$M(K_x, K_y, K_z, \ldots) = \lim_{n\to\infty} \frac{\mu^{(n)}}{B^{nd}} \quad . \tag{4}$$

This is the central formula of the present formalism as it yields the order parameter for arbitrary values of $\{K_\alpha\}$. To close the operational procedure we must now produce the RG recurrence equations for $\{K_\alpha\}$ and μ. We shall illustrate this for the anisotropic square lattice.

We shall adopt the cluster transformation[5] indicated in Fig. 1. The two-rooted graphs appearing therein are self-dual, and therefore very suited for the square lattice (as already proved in many other similar problems).

Before going on let us make a few comments concerning the divisor B^d appearing in Eq. (4). As we are in fact now replacing the Bravais lattice by an hierarchical one, this is a convenient place for stating that B^d will be approached by $B^{d_{bb'}}$ defined in what follows.

If we were interested only in the isotropic case ($J_x = J_y$) we would renormalize the two-rooted graph G (with chemical distance b between the roots; b = 3 for Fig. 1(b)) into the graph G' (with chemical distance b' between its roots; b' = 1 for Fig. 1(b), hence B = b/b' = 3). The graph G generates, through iteration, an

hierarchical lattice with intrinsic fractal dimensionality[6,7] $d_b = \ell nN_b/\ell nb$ ($d_b = \ell n9/\ell n3 = 2$ in Fig. 1(b)); analogously G' is to be associated with $d_{b'} = \ell nN_{b'}/\ell nb'$ ($N_{b'} = b' = 1$ in Fig. 1(b) which leaves indetermined $d_{b'}$; nevertheless it can be shown that the correct answer for this trivial case is $d_{b'} = 1$); N_b and $N_{b'}$ respectively are the number of bonds of graphs G and G'. It is convenient to define the dimensionality $d_{bb'}$, through

$$B^{d_{bb'}} \equiv N_b/N_{b'} \tag{5}$$

hence

$$B^{d_{bb'}} = b^{d_b}/b'^{d_{b'}} \tag{6}$$

hence

$$d_{bb'} = \frac{d_b \ell nb - d_{b'} \ell nb'}{\ell nb - \ell nb'} \tag{7}$$

Note that $d_{b1} = d_b$. If graphs G and G' have been consistently chosen to approximate the d-dimensional Bravais lattice, we must expect $\lim_{\substack{b\to\infty \\ b'<b}} d_{bb'} = \lim_{b\to\infty} d_b = d$.

In the anisotropic case (arbitrary J_x and J_y) we may extend definition (5) into

$$B^{d_{bb'}} \equiv \frac{N_b^x + N_b^y K_y/K_x}{N_{b'}^x + N_{b'}^y K'_y/K'_x} \tag{8}$$

where N_b^x and N_b^y ($N_{b'}^x$ and $N_{b'}^y$) are the numbers of bonds of G (G') respectively associated with K_x and K_y (K'_x and K'_y). Definition (8) recovers definition (5) in the following particular cases:

$(K_y/K_x, K'_y/K'_x) = (0,0)$, $(1,0)$, $(0,1)$ and $(1,1)$. Definition (8) is the simplest continuous expression which does so. Naturally other similar alternative definitions can be introduced for purposes we shall discuss later on. For example, for the q-satate Potts model, we can introduce

$$B^{d}_{bb'} \equiv \frac{N^x_b + N^y_b t_y/t_x}{N^x_{b'} + N^y_{b'} t'_y/t'_x} \tag{8'}$$

where the t's denote *thermal transmissivities*[8,9] defined through

$$t \equiv (1 - e^{-qk})/[1 + (q-1)e^{-qk}] \in [0,1] .$$

Let us now come back to the determination of the recurrences for $\{K_\alpha\}$ and μ for the q-state Potts ferromagnet. We impose that the correlation function between the two roots of the graphs must be preserved, i.e.

$$e^{-\beta\mathcal{H}'_{12}} = \operatorname*{Tr}_{3,4,5\ 6} e^{-\beta\mathcal{H}_{123456}} \tag{9}$$

where, in our case $(\sigma_i = 1,2,\ldots,q, \forall i)$,

$$-\beta\mathcal{H}'_{12} = qK'_x \delta_{\sigma_1,\sigma_2} + Ko \tag{10}$$

(Ko is an additive constant to be determined) and

$$-\beta\mathcal{H}_{123456} = qK_x(\delta_{\sigma_1,\sigma_3} + \delta_{\sigma_1,\sigma_6} + \delta_{\sigma_5,\sigma_6} + \delta_{\sigma_5,\sigma_2} + \delta_{\sigma_4\ \sigma_2})$$

$$+ qK_y(\delta_{\sigma_1,\sigma_6} + \delta_{\sigma_3,\sigma_5} + \delta_{\sigma_5,\sigma_2} + \delta_{\sigma_4,\sigma_6}) , \tag{11}$$

$\mathcal{H}'_{12}$ and $\mathcal{H}_{123456}$ respectively being the Hamiltonians of the small and large graphs of Fig. 1(b). Equation (9) uniquely determines

$$K'_x = f(K_x, K_y) \tag{12}$$

hence

$$K'_y = f(K_y, K_x) \tag{13}$$

where we have used the $x \leftrightarrows y$ invariance of our lattice.

Let us now establish the equation for μ by following along the lines of Ref. [4]. In order to break the symmetry we assume one of the roots of the graphs to be in a fixed state, say $\sigma_1=1$. We consider all possible configurations for the other sites, i.e., q (q^5) configurations for the small (large) graph, as well as the corresponding Boltzmann weights and the associated magnetic moments. The magnetic moment m associated with a given configuration is obtained by adding all site contributions, each of them being proportional to the *average coordination number*, defined by attributing to each bond a weight proportional to its coupling constant (if we adopt definition (8)), or analogously proportional to its transmissivity (if we rather adopt definition (8')); see Table 1 for the spin 1/2 Ising particular case ($q=2$). The present definition for *average* coordination number is the simplest continuous one which recovers that of the isotropic case (namely the standard coordination number) in both particular cases $K_y/K_x=1$ and $K_y/K_x=0$. Finally we impose, as we did in Eq. (1),

$$\langle m \rangle_{G'} = \langle m \rangle_G \tag{14}$$

where $\langle\cdots\rangle$ denotes the canonical thermal average. Eq. (14) has the form

$$\mu' = g(K_x,K_y)\mu \tag{15}$$

where $g(K_x,K_y)$ is a continuous function which satisfies $g(\infty,\infty) = B^{d_{bb'}} > g(0,0) > 0$. The determination of the function $g(K_x,K_y)$ demands the construction, for arbitrary q, of a table such as Table 1 where we must take into account the fact that the Potts order parameter is proportional to $(q\langle\delta_{\sigma_{i,1}}\rangle - 1)/(q-1)$. In general it is $g(K_x,K_y) \neq g(K_y,K_x)$ (e.g., the large cluster of Fig. 1(b) has five K_x-bonds but only four K_y-bonds). An undesirable consequence of this fact is that in general the present RG approximation will be not invariant under $K_x \rightleftarrows K_y$ permutation, as it should. The discrepancies are however very small (e.g., at most 3% between the q=2 cases for $K_y/K_x=0.5$ and $K_y/K_x=2$) and should vanish in the $b\to\infty$ limit.

Summarizing the method, to determine the spontaneous magnetization we are looking for, we have to use Eqs. (12), (13), (15) and

$$M(K_x,K_y,\ldots) = \lim_{n\to\infty} \frac{\mu^{(n)}}{B^{nd_{bb'}}} \tag{16}$$

which approximates Eq. (4). Equation (16) can alternatively be rewritten as follows:

$$M(K_x,K_y,\ldots) = \lim_{n\to\infty} \prod_{\ell=0}^{n-1} \frac{g(K_x^{(\ell)},K_y^{(\ell)},\ldots)}{B^{d_{bb'}}} \tag{17}$$

where we have used $\mu^{(o)}=1$ and $K_\alpha^{(o)} \equiv K_\alpha$ $(\alpha=x,y,\ldots)$. In the present application it is $B^{d_{bb'}} = 5+4K_y/K_x$.

III RESULTS

The results we have obtained for the spontaneous magnetization for q=1,2,3 and 4 are presented in Fig. 2 (isotropic case $K_y = K_x$) and Fig. 3 (anisotropic cases for typical values for the ratio $r \equiv K_y/K_x$). In Fig. 3(b) comparison is done with the exact answer[10], for intermediate temperatures and typical ratios the error is of the order of 10%. For the q=1 particular case we have presented, in Fig. 4, our results in the standard manner for bond percolation ($p_\alpha \equiv 1-e^{-K_\alpha}$ with $\alpha=x,y,...$) with $\eta \equiv (1-p_y)/(1-p_x)$; we have compared with other RG results[3], the exact answer being yet unknown.

In the neighbourhood of the critical point, the magnetization is given by $M \sim A(1-T/T_c)^\beta$. The present RG recovers the exact T_c for all (q,r) (this comes from our choice of *self-dual* graphs). The approximate exponent β is given[4] by

$$\beta = \frac{\ell n[B^{d_{bb'}}/g(K_c,K_c)]}{\ell n(df(K,K)/dK]_{K_c}} \quad ; \qquad (18)$$

β depends on q but not on the ratio $r(r\neq 0)$. This is as expected on the basis of universality arguments, and has been illustrated, for q=3, in Fig. 5. The numerical values for β are presented in Table 2 and compared with the exact results[11]. Though the numerical discrepancies are acceptable, we verify an incorrect tendency to increase (instead of decrease) for increasing q. However this error possibly disappears in the $b\to\infty$ limit, as verified in Ref. [4] for the isotropic case and b=2,3,4. The values we have obtained for A for typical values of (q,r) are indicated in Table 3. Comparison with exact results is possible only for q=2: the discrepancies are unexpectedly small.

IV CONCLUSION

A real space RG scheme has been formulated which, for the first time, enables a simple and direct calculation of the equation of states of *anisotropic* magnetic systems. It is based on the inspection of the spin configurations of small clusters, a fact which considerably helps intuition. The method is operationally as simple as a mean field calculation and can be used for arbitrary temperatures; the results are non trivial and can be systematically improved. At the microscopic level all quantities introduced vary softly with the external parameters such as temperature and anisotropy. Nevertheless, at the macroscopic level, the expected usual discontinuities, such as crossover phenomena, are satisfactorily described.

We illustrate the procedure through the calculation of the spontaneous magnetization of the q-state Potts ferromagnet in anisotropic square lattice, a problem which is yet unsolved for $q \neq 2$. We use the q=2 known exact results to test the quality of the method. Satisfactory agreement is obtained, specially for the critical amplitude. As a restriction we must mention that the present formalism shares with similar types of methods the not recovering of first order phase transitions which are known to occur for d=2 Bravais lattices for q high enough (in fact, q>4). To overcome this difficulty, an enlarged parameter space possibly needs to be introduced[12]. In any case the present results are correct for the hierarchical lattices which are used to approach the Bravais lattice under study.

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CAPTION FOR FIGURES AND TABLES

Fig. 1 - (a) The self-dual cell transformation used in the present RG to renormalize K_x (the arrows denote the "entrances" and "exits"). (b) the corresponding graphs G and G' (o and • respectively denote the roots and internal sites)

Fig. 2 - Magnetization as a function of the temperature for the isotropic case, for typical values of q.

Fig. 3 - Magnetization as a function of the temperature, for various ratios $r = K_y/K_x$: (a) q = 1; (b) q = 2 (the dashed curves are exact[10]); q = 3; (d) q = 4.

Fig. 4 - Probability P_∞ of a bond to belong to the infinite cluster as a function of the concentration $p_x \equiv 1 - e^{-J_x/k_BT}$ of "horizontal" bonds, for fixed $\eta = (1-p_y)/(1-p_x)$. For η = 0.5 and η = 1 we compare our curves with the results (dashed) of da Silva et al.[3]

Fig. 5 - q = 3 model. (a) Amplitude $A \sim M/(1-T/T_c)^\beta$ as a function of the temperature, for typical values of $r \equiv K_y/K_x$ ($T_{crossover}$ is defined through the construction indicated by thedashed lines). (b) Dependence of $T_{crossover}$ on the ratio $r \equiv K_y/K_x$

Table 1 - Estabishement of eq. (14) for the anisotropic Ising ferromagnet (q = 2). We have used

$\mathcal{H} = -\sum_{<i,j>} J_{ij}\sigma_i\sigma_j (\sigma_i = \pm 1)$ rather than

$\mathcal{H} = -q \sum_{<i,j>} J_{ij}\delta_{\sigma_i,\sigma_j} (\sigma_i = 1,2,\ldots q)$

(a) $\langle m \rangle_{G'} = 2\mu' e^{K'_x}/(e^{K'_x} + e^{-K'_x})$

(b) Only 7 among $2^5 = 32$ possible configurations have been represented: $\langle m \rangle_G = (e^{5K_x + 4K_y}(10 + 8K_y/K_x) +$

$2e^{K_x}(6 + 4K_y/K_x) + 2e^{3K_x+2k_y}(8 + 6K_y/K_x) +$

$e^{K_x+2K_y}(6 + 6K_y/K_x) + e^{-3K_x-2K_y}(-2-2K_y/K_x) + \ldots)\mu/$

$(e^{5K_x+4K_y} + 2e^{K_x} + 2e^{3K_x+2K_y} + e^{K_x+2K_y} + e^{-3K_x-2K_y} + \ldots)$

Table 2 - Present RG results for the critical exponent β and the corresponding exact values.

Table 3 - Present RG results for the amplitude A of the magnetization (the exact values for q=2 are presented between parentheses). In the q = 0 limit, due to precision limitations we cannot affirm that A is independent of r.

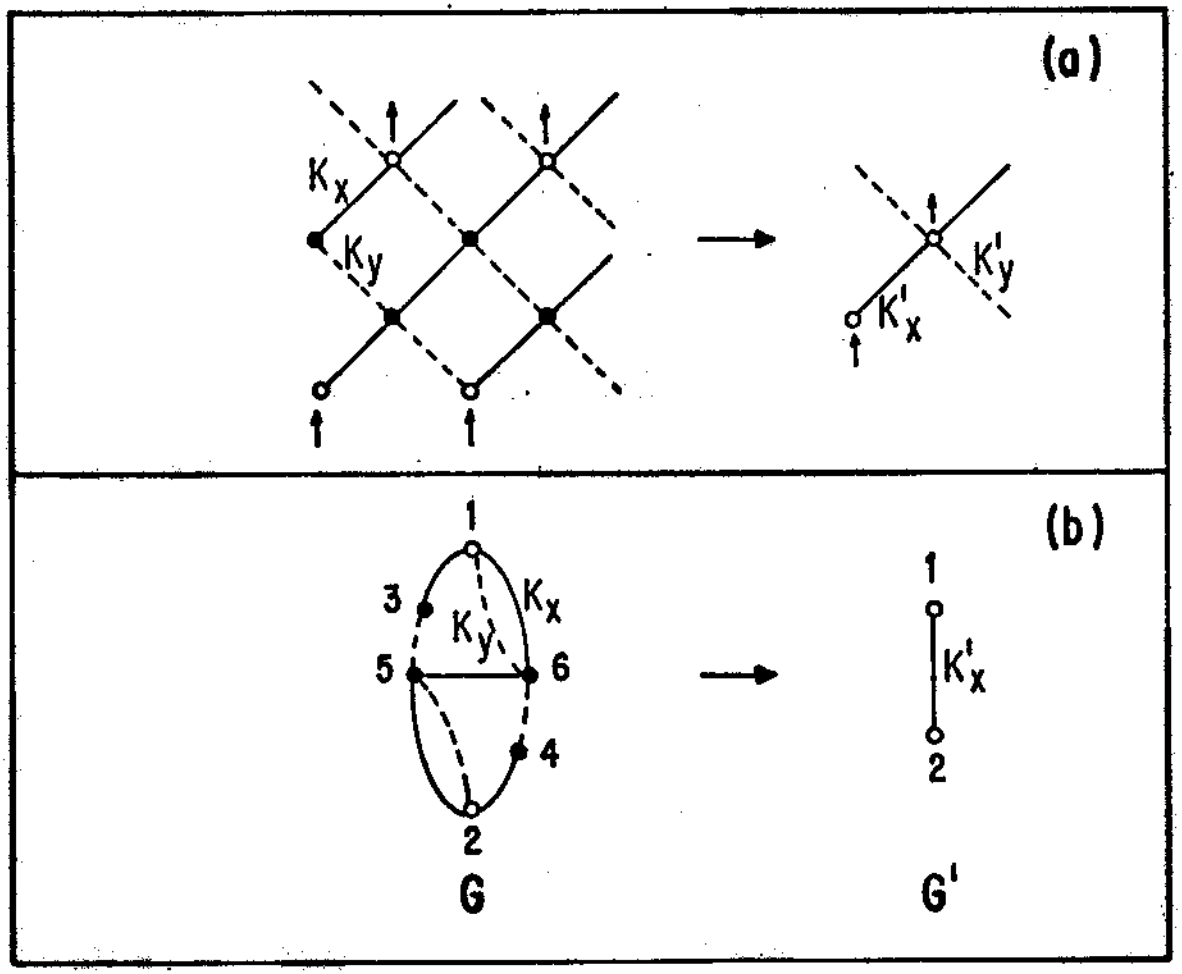


FIG.1

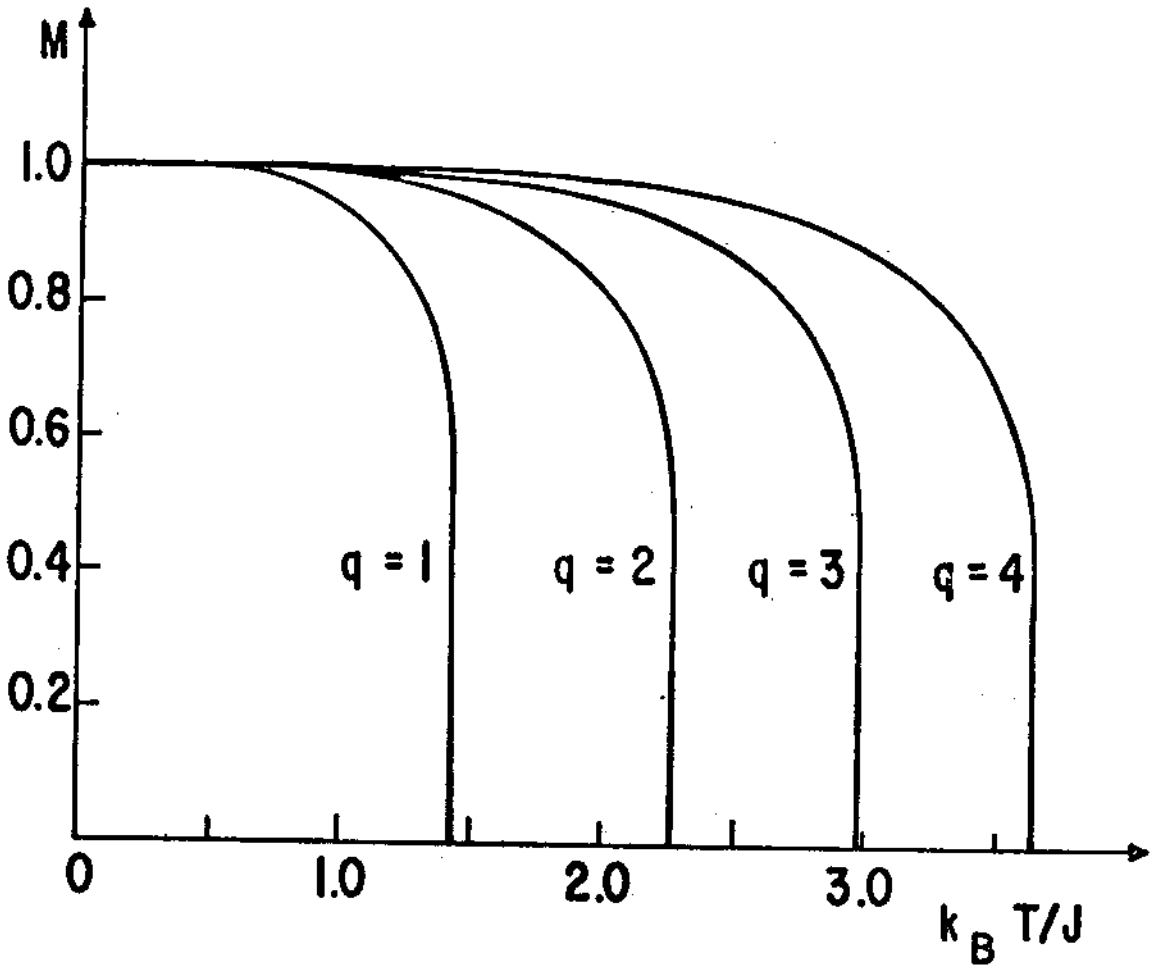


FIG. 2

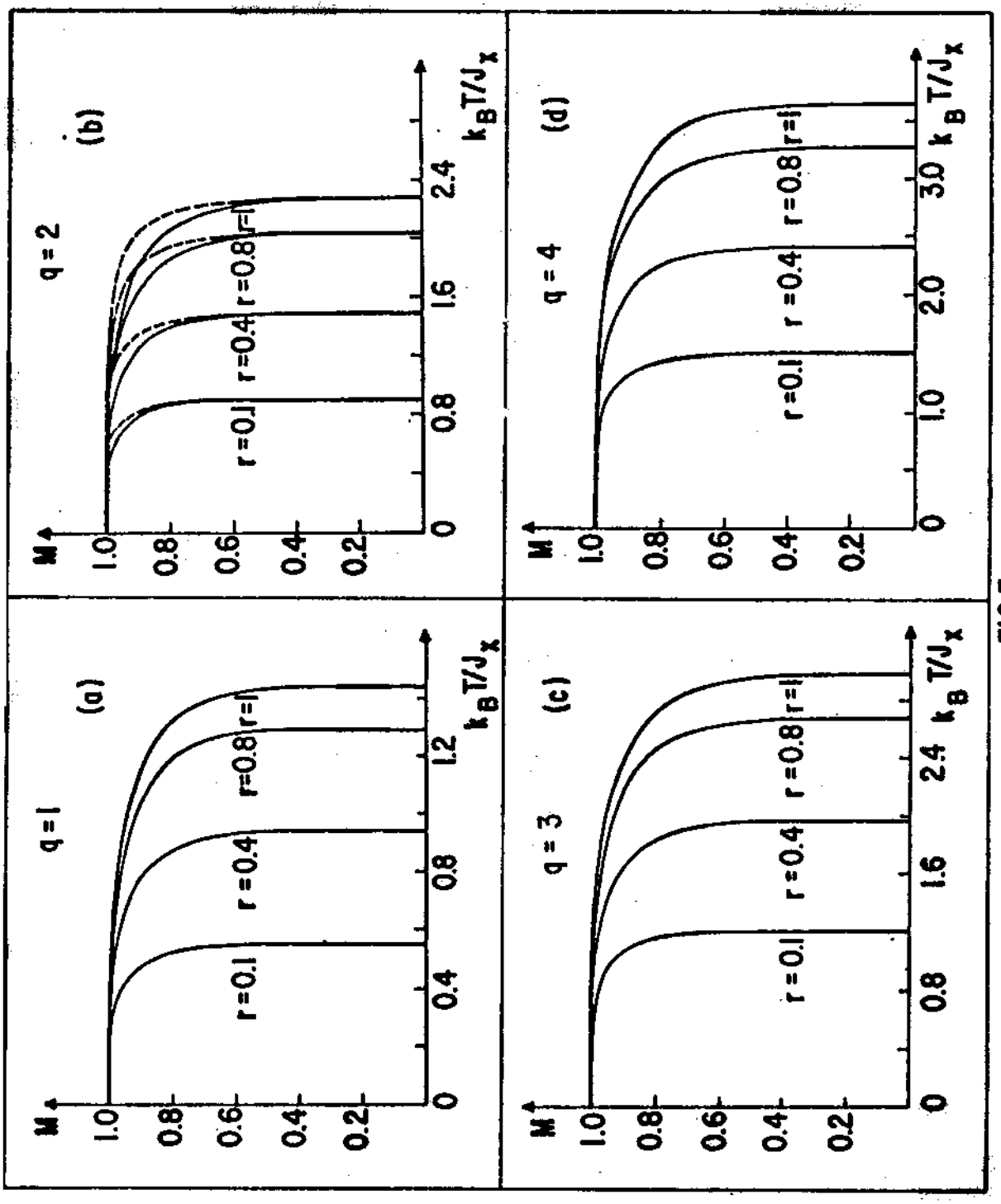

q = 1
(a)
M
1.0
0.8
0.6
0.4
0.2
0
0.4
0.8
1.2
$k_B T/J_x$
r=0.1
r = 0.4
r=0.8
r=1
q = 2
(b)
M
1.0
0.8
0.6
0.4
0.2
0
0.8
1.6
2.4
$k_B T/J_x$
r=0.1
r=0.4
r=0.8
r=1
q = 3
(c)
M
1.0
0.8
0.6
0.4
0.2
0
0.8
1.6
2.4
$k_B T/J_x$
r=0.1
r = 0.4
r=0.8
r=1
q = 4
(d)
M
1.0
0.8
0.6
0.4
0.2
0
1.0
2.0
3.0
$k_B T/J_x$
r=0.1
r = 0.4
r=0.8
r=1

FIG.3

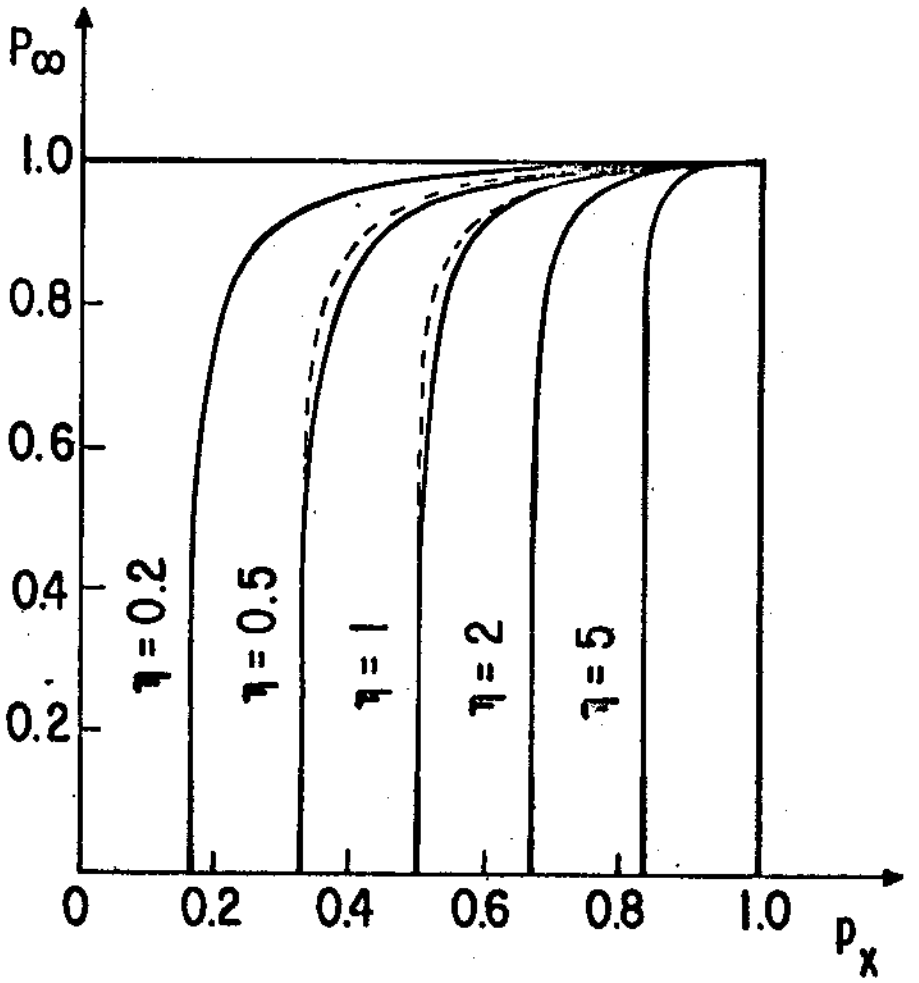

P_∞
1.0
0.8
0.6
0.4
0.2
$\eta = 0.2$
$\eta = 0.5$
$\eta = 1$
$\eta = 2$
$\eta = 5$
0
0.2
0.4
0.6
0.8
1.0
p_x

FIG. 4

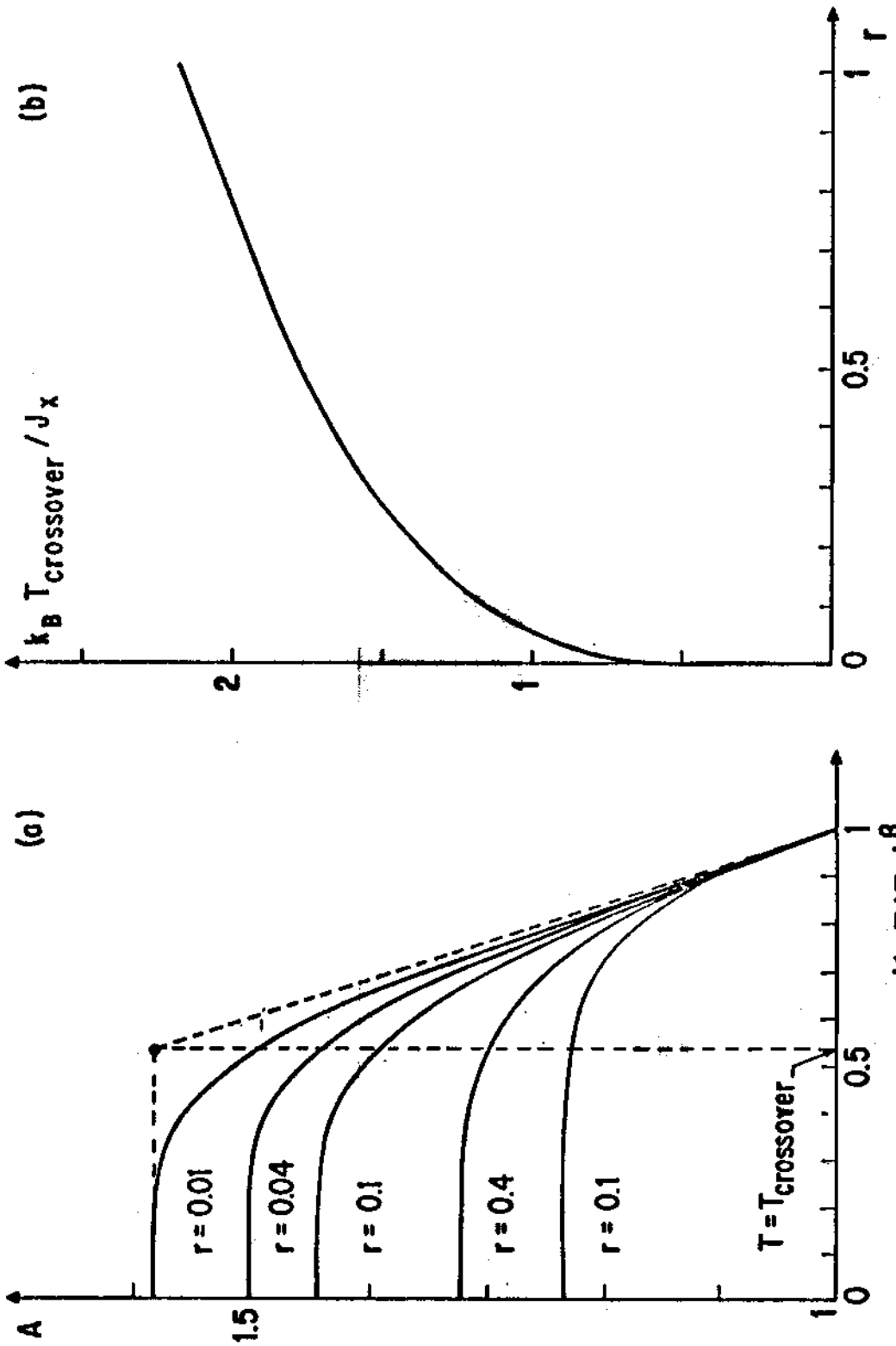

(a)
A
1.5
1
r = 0.01
r = 0.04
r = 0.1
r = 0.4
r = 0.1
T = T_crossover
0
0.5
1
(1-T/T_c)^β
(b)
k_B T_crossover / J_x
2
1
0
0.5
1
r

FIG.5

(a) G' configuration	weight	m
	$e^{K'_x}$	$2\mu'$
	$e^{-K'_x}$	0

TABLE 1

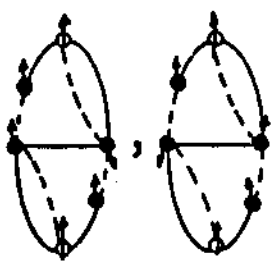
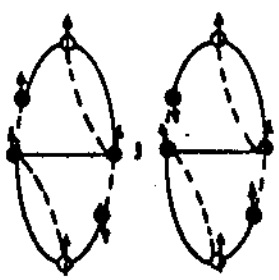
(b) G configuration	weight	m
	$e^{5K_x + 4K_y}$	$(10 + 8K_y/K_x)\,\mu$
	e^{K_x}	$(6 + 4K_y/K_x)\,\mu$
	$e^{3K_x + 2K_y}$	$(8 + 6K_y/K_x)\,\mu$
	$e^{K_x + 2K_y}$	$(6 + 6K_y/K_x)\,\mu$
	$e^{-3K_x - 2K_y}$	$(-2 - 2K_y/K_x)\,\mu$

TABLE 1

q	β(RG)	β(exact [11])
0	0.10	1/6 ≃ 0.167
1	0.152	5/36 ≃ 0.139
2	0.168	1/8 ≃ 0.125
3	0.178	1/9 ≃ 0.111
4	0.187	1/12 ≃ 0.0833
∞	ℓn(9/5)/ℓn5 ≃ 0.365	—

TABLE 2

r \ q	0	1	2	3	4
1	1.1	1.17	1.21 (1.22)	1.24	1.26
0.8	1.1	1.18	1.22 (1.22)	1.26	1.28
0.4	1.1	1.21	1.28 (1.23)	1.32	1.37
0.1	1.1	1.27	1.37 (1.26)	1.44	1.51

TABLE 3

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